Development of a reduced chemical mechanism targeted for a 5-component gasoline surrogate: A case study on the heat release nature in a GCI engine

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Abstract:

Gasoline Compression Ignition (GCI) is a promising engine operating mode that can reduce maximum pressure rise rate (MPRR) without knock tendency and better control the combustion phasing compared to the Homogeneous Charge Compression Ignition (HCCI) by using a late direct-injection (DI). In this study, a 107-species reduced mechanism and a 207-species skeletal mechanism were developed using the Computer Assisted Reduction Mechanism (CARM) and validated under engine conditions for a newly developed 5-component surrogate for a Haltermann 437 certification gasoline (AKI=93). Then, 3D computational fluid dynamics (CFD) simulations with an optimized grid size determined by a grid convergence study were performed with the 107-species reduced mechanism and the 5-component certification gasoline surrogate. Two experimental boosted GCI cases with similar, moderate MPRR and heat release parameters, but different second DI timings (-52° aTDC and -5° aTDC), were validated and analyzed. For the -52° aTDC DI case, the combustion can be interpreted as a partially sequential auto-ignition due to the competition between the charge cooling effect and the equivalence ratio (ϕ)-sensitive effect of the stratified mixture, which is responsible for mitigating the MPRR. For the -5° aTDC DI case, the combustion can be decoupled into a partially sequential auto-ignition and a subsequent non-premixed combustion by the DI fuel near top dead center in the compression stroke. The MPRR is relaxed through the slow, mixing-limited combustion between the injected fuel and the premixed mixture.

Keywords: Mechanism; Reduction; Surrogate; Stratification; GCI

Nomenclature (Definitions, Acronyms, Abbreviations)

AKI: anti-knock index
AMR: adaptive mesh refinement
aTDC: after top dead center
CA10: crank angle where 10% cumulative heat release occurs
CARM: computer assisted reduction mechanism
CSP: complete stoichiometric products
DI: direct injection
DHA: detailed hydrocarbon analysis
DNS: direct numerical simulation
DRGEP: direct relation graph with error propagation
EGR: exhaust gas recirculation
GCI: gasoline compression ignition
HCCI: homogenous charge compression ignition
IVC: intake valve closing
MHRR: maximum heat release rate
MON: motor octane number
MPRR: maximum pressure rise rate
NTC: negative temperature coefficient
PFI: port fuel injection
QSSA: quasi-steady-state assumption
RANS: Reynolds averaged Navier-Stokes
RCM: rapid compression machine
RON: research octane number
SODI: start of direct injection
 t_{ign} : auto-ignition delay time
TSA: target search algorithm
TCI: turbulence-chemistry interaction
WMR: well-mixed reactor
 ϕ : equivalence ratio

1. Introduction

Next-generation engine operating strategies aim to increase efficiency in gasoline-fueled engines by moving away from traditional spark-ignition (SI) engines towards higher compression ratio, premixed or partially premixed, compression-ignition (CI) engines. Homogeneous Charge Compression Ignition (HCCI) is a low temperature

combustion mode that has attracted substantial research attention because of the great potential to achieve low emissions and high efficiency [1]. However, HCCI is limited at high loads due to the strong knock or ringing tendency by the extremely rapid combustion [1, 2]. Therefore, a lean mixture or high exhaust gas recirculation (EGR) levels are necessary to reduce the maximum heat release rate (MHRR) and maximum pressure rise rate (MPRR) to acceptable levels [1]. Additionally, the lack of direct in-cycle control of combustion phasing is another challenge that makes HCCI unlikely to be a practical engine mode for the entire operation [3].

In the last decade, many new concepts for a gasoline-fueled CI engine have been developed that aim to reduce the MPRR by using fuel stratification to prolong the combustion duration, such as Gasoline Compression Ignition (GCI) [4], Gasoline Direct Injection Compression Ignition [5], Partial Fuel Stratification [6], Stratified Charge Compression Ignition [7], and Partially Premixed Combustion [8], among others. The fuel stratification in these concepts is mainly accomplished by mixing the majority of the fuel with air during the intake stroke and direct injecting the rest during the compression stroke. In this paper, GCI will be used to represent this concept. Unlike HCCI, the late injection timing in GCI can be used to control the combustion phasing. The inhomogeneity introduced by the late injection influences the start of combustion and facilitates a sequential auto-ignition that reduces MPRR [9]. The sequential ignition behavior in GCI depends on how the fuel auto-ignition characteristics change with equivalence ratio (ϕ) and if the fuel exhibits single or multi-stage ignition [9]. The ϕ -sensitivity is an indicator that describes how a fuel will respond to stratification (a fuel is ϕ -sensitive if increasing ϕ changes the combustion phasing) [10]. Use of a ϕ -sensitive fuel in GCI can moderate the MHRR and MPRR, thus increasing the maximum operating load limit of GCI compared to HCCI. The use of GCI has resulted in up to 26% less fuel consumption than the traditional SI mode in a light duty engine [11, 12] and up to 56% indicated thermal efficiency in a heavy duty engine [13]. However, fuels with high RON which have long ignition delay times [14], sometimes are more difficult to auto-ignite which may lead to misfire at starting and low loads. It has been proposed that the optimum fuel RON for GCI is in the range of 70 to 85, which would have longer ignition delay time than diesel fuel and avoid instability at low loads [15, 16]. Additionally, unburned hydrocarbon emissions are another issue to be considered [15].

Computational fluid dynamics (CFD) simulations of GCI require the identification of a gasoline surrogate fuel that sufficiently reproduces the physical and chemical properties of the real fuel [15, 17]. A candidate gasoline surrogate should be able to account for the distillation curve (component molecular weights), H/C ratio, RON, fuel sensitivity, stoichiometric A/F ratio, etc. [18, 19]. When aromatics and olefins exist in the real fuel, a primary reference fuel (PRF; iso-octane and n-heptane mixture) is not a suitable fuel surrogate because the ignition characteristics of the fuel are not well-reproduced for a broad range of engine-relevant conditions due to the strong impact of unsaturated components on the sensitivity of gasoline fuels [18]. Therefore, gasoline surrogates should be comprised of additional components beyond iso-alkanes and n-alkanes to more accurately represent the fuel reactivity over a broad range of conditions.

Detailed reaction mechanisms developed for hydrocarbon oxidation covering a large range of conditions can have thousands of species for heavy fuels [20], which are prohibitively large for use in 3D-CFD simulations in terms of the CPU time. For this reason, there is great interest in reducing the size of the detailed mechanisms while maintaining sufficient species and reaction steps to adequately reproduce relevant physical phenomena at given target conditions, such as ignition delay time and laminar flame speeds at engine-relevant temperatures and pressures.

In this paper, the Haltermann 437 certification gasoline with better performance for resisting knock (AKI=93), which is different from the characteristics of gasoline fuels studied before such as the RD387 (AKI=87) [21], is utilized for exploring the effect of fuel on the sequential ignition and knock mitigation in a GCI engine. A novel 5-component surrogate for the Haltermann 437 certification gasoline is developed. Then, a 107-species reduced mechanism and a 207-species skeletal mechanism for the 5-component gasoline surrogate are reduced from an updated version of the 1389-species detailed gasoline surrogate mechanism by Lawrence Livermore National Laboratory (LLNL) [20]. By coupling the chemistry model developed, 3D-CFD simulations are conducted to clarify previous experimental observations of the heat release behavior for two specific GCI cases [22], which have similar MPRR and heat release parameters but very different second injection timings.

2. Fuel surrogate formulation for Haltermann 437 certification gasoline

In the GCI experiments [22] to be computationally analyzed in this study, the Haltermann 437 certification gasoline is used. The typical properties of it are shown in Table 2 and more information can be found in the appendix of [23]. Due to the aforementioned necessity on multi-component surrogates, the methodology proposed by Mehl et al [18] is applied based on the specifications of the fuel. In the approach, two correlations calculated from experimentally measured data at 25 atm are used to define the relations between the auto-ignition properties and the key index such as antiknock index (AKI) and sensitivity (=RON-MON). One is between the sensitivity and the slope of the negative temperature coefficient (NTC) region, the other is between the AKI and the ignition delay time at 825 K. To formulate a suitable palette of components for the surrogate, iso-octane, n-heptane and toluene are first selected to represent the classes of iso-alkanes, n-alkanes and aromatics. Olefins are excluded due to the negligible concentration in the fuel. From the detailed hydrocarbon analysis (DHA) by the method of ASTM D6733, iso-pentane and n-pentane are two major iso-paraffin components apart from iso-octane with 18.0% and 3.1% by volume, respectively. Thus these two compounds are included to form the final 5-component surrogate model. Finally, these components are blended to reach the percentage values shown in Table 1 by matching the index in Table 2 as well as the stoichiometric air/fuel ratio.

Table 1

Surrogate formulation

Table 2

Typical properties of Haltermann 437 gasoline and its surrogate

3. Chemical mechanism reduction implementation

The associated detailed mechanism from Lawrence Livermore National Laboratory (LLNL) [20] has been updated with 52 refined rate constants and 30 additional reaction steps to more accurately represent the Haltermann 437 certification gasoline surrogate chemistry with 1389 species and 5962 reactions. Due to the use for CI engine conditions, NO_x species and related reactions extracted from GRI-2.11 [24] were added to the

detailed mechanism, increasing the number of species to 1393 (addition of N, NO, NO₂, and N₂O) and the number of reaction steps to 5976.

In the reduction implementation for the Haltermann 437 certification gasoline, the newly developed 5-component surrogate is targeted under 13 GCI engine-relevant conditions. The details of the target conditions considered in this study are shown in Table 3. Considering the nature of GCI combustion, auto-ignition delay time (t_{ign}) defined with 400 K increase is evaluated with an in-house Well-Mixed Reactor (WMR) model [25]. The Computer Assisted Reduction Mechanism (CARM) [26] is a computer code that automates the process of mechanism reduction using algorithms developed in the research group of Chen [27-30] and others [31, 32]. Due to the efficient characteristics, the direct relation graph with error propagation (DRGEP) based approach using Dijkstra search algorithm, which has proved to be more accurate on species removal than the other search algorithms by Niemeyer and Sung [32], is used for the first-step reduction. From previous studies of other researchers [33, 34], the DRGEP-based methods are very sensitive to the target species such as HO₂, CO, CH₂O, etc. near NTC regions for two-stage ignition fuels. Thus HO₂ and CH₂O are targeted with the 5-component surrogates, O₂, N₂, H₂O and CO₂. Additionally, NO is added to the target species list for keeping the paths related to it. After three-round restart running of the DRGEP-Dijkstra method, a 720-species skeletal mechanism is generated with the worst-case relative error of 4.1% among the 13 target cases. Then a trial-and-error method, Targeted Search Algorithm (TSA) [29], is used to systematically test species for removal from the 720-species skeletal mechanism. In the TSA, the species in the original mechanism are tested for removal in ascending order by maximum mole fraction at a given target condition. After the removal of each test species and any associated reactions, the relative error of the new mechanism is compared to the detailed mechanism by running flame codes at each target condition. If the relative error does not exceed pre-defined thresholds, the tested candidate will remain removed from the mechanism; otherwise, the species and reactions are not removed from the mechanism. After 10 rounds of restarting TSA with gradually increasing thresholds to 12% (rel.) and 0.1 μ s (abs.) for t_{ign} , the final skeletal mechanism reaches 207 species and 1026 reactions with maximum relative error of 11.3% for the target cases. However, the size of the 207-species skeletal mechanism is still unacceptable for 3D-CFD simulations in engine industry. Therefore, the quasi-steady state assumption (QSSA) [27, 28] is applied to certain intermediate species

to further reduce the skeletal mechanism. In the CARM, quasi-steady state (QSS) species are identified by evaluating the level of concentration with the help of a production rate analysis. After determining the QSS species group, independent elementary reactions are selected to remove the QSS species for systematic construction of the reduced mechanism. Finally, a 107-species reduced mechanism comprising of 102 steps is developed and 100 QSS species are obtained.

Table 3

Target conditions in mechanism reduction for GCI engine simulation.

4. Validation of the skeletal and reduced mechanism

The developed 107-species reduced and 207-species skeletal mechanisms are validated against the detailed mechanism for t_{ign} under a wide range of conditions. Overall, there is good agreement between them at $\phi=0.3-2.0$, $P=20-80$ bar, and $T=625-1300K$ for the 5-component gasoline surrogate. In Fig. 1(b), a comparison between rapid compression machine (RCM) experimental data from [23] and simulated t_{ign} (constant volume and adiabatic assumption) using the three mechanisms for the Haltermann 437 gasoline at $P=50$ bar is presented. The skeletal and reduced mechanisms predict very similar t_{ign} compared to the detailed mechanism, and all the three mechanisms exhibit good predictions compared to the RCM experiments although there is no experimental information against which rich mixtures can be validated. In Figs. 1(a) and 1(c), mechanism validation at other conditions for the certification gasoline are plotted with good agreement. The files of the 107-species reduced mechanism with both FORTRAN 77 and C versions, the 207-species skeletal mechanism, and the updated version of the detailed mechanism of [20] are provided in the supplemental materials.

Fig. 1. Comparison of t_{ign} between the detailed mechanism, 207-species skeletal mechanism and the 107-species reduced mechanism using the 5-component Haltermann 437 certification gasoline surrogate under the pressure of (a) 20 bar, (b) 50 bar and (c) 80 bar. Experimental data of (b) is in [23].

5. GCI engine experiments and simulation setup

The Reynolds Averaged Navier-Stokes (RANS) based CFD software of CONVERGE [35] were applied to simulate three-dimensional reactive flow with moving boundaries for the MIT GCI engine [22]. Fig. 2 shows the computational mesh and Table 4 lists the engine specifications. In order to match the motored pressure traces, the effective compression ratio in the computation study is tuned to 15.16:1 (increased from 15:1). Simulations are computed from intake valve open to exhaust valve open. Turbulence is modeled using the RNG $k-\varepsilon$ approach [36]. The newly developed 107-species reduced mechanism is employed for the chemistry model by modifying the user-defined function module. The Haltermann 437 certification gasoline used in the MIT two-injection GCI experiments [23] is represented by the aforementioned 5-component surrogate. The first injection in the experiments by a port fuel injection (PFI) is assumed to form a premixed charge since it occurs at -290° aTDC during the intake stroke. A 5-hole centrally mounted GDI injector with hole diameters of $200\ \mu\text{m}$ is used for the direct injection (DI) during the compression stroke (the injection pressure was 490 bar). The orifice orientation angle relative to the injector axis is 75° . The injection process is modeled by a Lagrangian spray model and a stochastic collision model with the Rosin-Rammler distribution [37]. The Kelvin-Helmholtz Rayleigh-Taylor (KH-RT) model is chosen to simulate the breakup of the liquid fuel droplets [38]. The experimental coolant temperature is used for the constant temperature boundary conditions, except for the piston that was set 100°C higher. The wall heat transfer model by Han and Reitz [39] is selected to account for the heat loss to the wall.

Fig. 2. Computational mesh of the MIT GCI engine at -6° aTDC.

Table 4

Engine specifications in the experiment.

In the experiments [22], a PFI provides an almost homogeneous background charge with 60% of the total fuel. The remaining 40% of the total fuel is injected as a late DI at different start of direct injection (SODI) timings to offer different scales of stratification. In Fig. 3, the experimental data of the MPRR changing with the second DI timing is plotted [22]. As the SODI timing in the experiments was retarded from the early compression, the

MPRR drops first, then increases strongly, and finally decreases again. Interestingly, there are two cases with quite different SODI timings of -52° aTDC and -5° aTDC during the compression stroke, but with similar CA10, CA50 and MPRR (The CA10 and CA50 are defined as the crank angles of 10% and 50% of cumulative heat release, respectively). Because the different SODIs correspond to different levels of stratification, yet the MPRR is the same at similar CA10 and CA50, the authors [22] proposed that the heat release process was mostly a bulk process instead of a sequential process. However, NO_x emissions measurements in the experiment were much higher for the later injection timing of SODI = -5° aTDC compared to SODI = -52° aTDC, which suggests that the combustion may be at least partially non-premixed (mixing-limited) for SODI = -5° aTDC. Consequently, the current study employs 3D-CFD simulations to clarify these observations.

Fig. 3. MPRR as a function of the SODI in the MIT experiments [22].

The total fuel mass injected for the cycle was 23 mg and the EGR level was 15% at $P_{in}=1.8$ bar in the experiments. As a result, the global $\varphi=0.25$ for the premixed charge increased to $\varphi=0.41$ after the DI. Herein, the equivalence ratio is calculated without including the EGR. In the discussion section, a local cell equivalence ratio will be provided to analyze the transient combustion process. The DI duration was 0.39 ms (2.8°CA) and the injection pressure was 490 bar. Complete stoichiometric products (CSP) were used to simulate EGR with N_2 , CO_2 and H_2O in proportions resulted from complete stoichiometric combustion of the fuel with air. Sjöberg et al. [40] compared the effect of different degrees of the real EGR and the CSP on the CA10 under gasoline HCCI combustion. The results indicate that the main difference between the real EGR and the CSP is the presence of the trace species by the incomplete combustion, and the real EGR tends to advance the ignition timing by less than 2° due to the new pathways by the partially oxidized fuel. Therefore, the CSP is widely employed to explain the effects of EGR, especially when the EGR ratio is relatively low [6, 21].

6. Grid convergence and validation

Compared to the direct numerical simulation (DNS) that resolves all scales down to the Kolmogorov scale, the smallest length scales in a RANS simulation are significantly larger by introducing enhanced turbulent diffusion

coefficients for momentum, species, and energy. In a DNS simulation, all length scales are supposed to be resolved to be accurate. In a similar manner, all RANS length scales should be resolved as well. However, it is common with under-resolution in RANS simulations. The under-resolved scales may bring significant sub-grid terms, which have an adverse impact on the simulation results. In order to ensure that all scales can be resolved with sufficient resolution in RANS simulations, grid convergence studies must be conducted to examine the effect of sub-grid RANS fields on the turbulent combustion results. With a view to the tradeoff between the mesh resolution and simulation time, adaptive mesh refinement (AMR) is a well suited tool to efficiently place grid cells, and flexibly adding embedment to the regions where the flow field is most under-resolved or where the sub-grid fields are unacceptably large. In RANS, the AMR can be expressed by Eqs. (1)-(3):

$$\overline{f''} = \bar{f} - \bar{f}' \quad (1)$$

$$\overline{f''} = -\alpha_{[k]} \frac{\partial^2 \bar{f}'}{\partial x_k \partial x_k} \quad (2)$$

$$dx = \frac{dx_{base}}{2^n} \quad (3)$$

where $\bar{f}$ and $\bar{f}'$ are the actual and resolved scalar fields, respectively. The $\overline{f''}$ is the sub-grid scalar field, which can be approximately evaluated by a 2nd order term in the series in Eq. (2), where $\alpha_{[k]}$ is $dx_k^2/24$ for a rectangular cell and the bracket indicates no summation. A cell will be embedded if the absolute value of the sub-grid field in Eq. (2) exceeds a user specified value. Then the AMR method described above properly refines cells in the corresponding regions with the expression in Eq. (3), where dx_{base} and n are the base grid cell size and embedded level in the simulation. dx is the reference minimum cell sizes in AMR.

In this work, the case with SODI at -5° aTDC is used for grid convergence due to more complicated activities than the other SODI case. The AMR is employed from -20° aTDC to 30° aTDC for the temperature and velocity fields with sub-grid criterion of 2.5 K and 1 m/s, respectively. The base grid cell size is set to be 2 mm, and the minimum cell size when AMR works is investigated in the range of 2 mm ($n=0$), 1mm ($n=1$), 0.5 mm ($n=2$), and 0.25 mm ($n=3$). In Fig.4, the enhanced mesh resolution by AMR with level 2 ($dx=0.5$ mm) is plotted for the case with SODI at -5° aTDC. By the strong temperature and velocity gradient after the injection, the refined grids

mainly appear in the region of spray plumes at this moment. In the grid convergence study, when the simulated results are not changing significantly with increasing grid resolution, it indicates that the field is well resolved and the sub-grid field is no longer important. To implement it, the in-cylinder pressure profile is matched with the experimental data in Fig. 5 by altering the inflow boundary temperature condition for the case with AMR level of 2 first. Because of the EGR effect, the inflow boundary temperature is tuned to 390 K instead of the experimental intake temperature of 353 K. Then all the cases of different AMR levels are tested with the same setting. Fig.5 shows the in-cylinder pressure and heat release rate traces changing with varying levels of AMR. As can be seen in this figure, the minimum mesh resolutions of 0.5 mm and 0.25 mm are quite similar, but the other two coarse grid sizes behave with a much earlier ignition, which means the sub-grid terms are not important when the minimum mesh resolution reaches 0.5 mm. This conclusion is the same for engines with similar bore diameters in [41, 42]. It is noted that the turbulence chemistry interaction (TCI) model [43, 44] is not considered for turbulent mixing in this study. However, Pomraning et al. [41] shows that accurate turbulent combustion results can be obtained using a RANS model with AMR and detailed chemistry without TCI model if sufficient mesh resolution is applied.

Fig. 4. AMR (level=2, base grid size=2 mm) enhanced mesh resolution in the slice located at 1.7 mm below the cylinder head at -2° aTDC for the case with SODI at -5° aTDC.

Fig. 5. In-cylinder pressure and heat release rate traces with varying mesh resolution for the case with SODI at -5° aTDC.

Comparison of in-cylinder pressure versus crank angle between the experiment and simulation is shown in Fig. 6. Herein, the case of SODI = -52° aTDC uses a fixed grid refinement with level 2 in Eq. (3) in the region of spray plumes from -52° aTDC to -32° aTDC. Additionally, AMR with level 2 is employed from -20° aTDC to 30° aTDC. Fig.6 shows that there is satisfactory agreement for the two SODIs considered. Table 5 shows the

experimental and numerical values of heat release parameters, MPRR, and NO_x . The simulation can predict these key parameters very well.

Fig. 6. In-cylinder pressure as a function of crank angle for the simulation and experiment.

Table 5

Heat release parameters, MPRR, and NO_x emission data validation

7. Results and discussion

In order to better understand the observed results, the ϕ -sensitivity of the certification gasoline surrogate was determined using an in-house single-zone Well-Mixed Reactor (WMR) engine code [25] with the reduced and detailed mechanisms. In the simulation, the temperature and the pressure at the intake valve closing (IVC) timing are fixed at 376 K and 1.8 bar to elucidate the effect of equivalence ratio on CA10, which is considered as the start of combustion. The ϕ -sensitivity (CA10 vs. ϕ) is presented in Fig. 7. It can be seen that the CA10 advances as ϕ increases for both the reduced and detailed mechanisms. Thus, the certification gasoline is ϕ -sensitive at these conditions, although the effect is not as strong as RD387 gasoline [9] due to the weaker pre-ignition heat release at the pressures considered. In GCI, the inhomogeneity introduced by the late injection will facilitate a sequential auto-ignition that reduces MPRR if the fuel is ϕ -sensitive [45]. However, the weak ϕ -sensitivity of the certification gasoline surrogate may limit the degree of sequential auto-ignition.

Fig. 7. CA10 vs. equivalence ratio under fixed IVC temperature and boosted pressure (1.8 bar) for the certification gasoline surrogate with the 107-species reduced mechanism and the 1393 species detailed mechanism, calculated by a single-zone WMR engine code.

Further analysis of the in-cylinder ϕ and thermal stratification is performed to better understand the reasons behind the similar observed MPRR for the two SODI considered. In Fig. 8, the local ϕ - T map is plotted with three

different crank angles for the case of SODI = -52° aTDC. The local ϕ in the cell is given as:

$$\phi = \frac{2 \sum N_i \eta_{C,i} + 0.5 \sum N_i \eta_{H,i}}{\sum N_i \eta_{O,i}} \quad (4)$$

where N_i is the number of moles of species i and $\eta_{C,i}$, $\eta_{H,i}$, and $\eta_{O,i}$ are the number of carbon, hydrogen and oxygen atoms, respectively, for species i . Each scatter in the plots represents the thermochemical state in each of the cells representing the cylinder. In each figure, the mole fraction of OH radical, which is treated as the indicator of high temperature heat release during combustion processes, is plotted with contours to show the heat release sequence.

In Fig. 8(a) at -3° aTDC, the highest OH appears in the region of the leanest mixture with the highest local temperature. It indicates that the mixture with the weakest mixing between the PFI and DI ignites first. Stronger mixing with the fuel from DI reduces the temperature by charge cooling effect. The resultant increase of ignition delay maintains a relatively low OH mole fraction in richer mixture regions despite the ϕ -sensitivity in homogeneous conditions favoring a shorter ignition delay as the mixture is enriched (Fig. 7).

In Fig. 8(b), at 2° aTDC there is predicted to be two regions with the highest mole fraction of OH radicals. As in Fig. 8(a), region 1 in Fig. 8(b) shows early heat release because the local temperature remains high as a result of little charge cooling via DI. Region 2 also exhibits a simultaneous, early heat release in slightly richer compositions, despite there being a marginally lower local temperature, as a consequence of the ϕ -sensitivity characteristics. Further details at this crank angle are shown in Figs. 9 and 10 with iso-surface plots for OH mole fraction and equivalence ratio. In Fig. 9, high OH mole fraction of 7.8×10^{-7} in red is sampled to locate the two regions in Fig. 8(b). In the left plot, $\phi = 0.43$ in blue and 0.52 in cyan are selected for the typical values in regions 1 and 2, respectively. $\phi = 0.47$ in blue is plotted in the right figure to represent the hiatus region in Fig. 8(b). Based on the intersection between the OH mole fraction and equivalence ratio iso-surfaces in the left plot, the lower red region is region 1 with little effects by the DI, and the upper red region stands for region 2 with higher equivalence ratio by mixing charge from DI. Although it looks indistinct, there is no intersection in the right figure, thus forming the hiatus region of Fig. 8(b). By plotting with the same setting apart from a lower value

of OH mole fraction ($6.5e-7$) in yellow, the right figure of Fig. 10 shows that the intersection is in the lower yellow area.

In Fig. 8(c) at 4° aTDC of CA10, ultimately the high OH mole fractions are associated with richer compositions, reflecting the development of combustion from remarkably lean mixtures ($\phi < 0.45$) to somewhat richer zones as the crank angle advances. Consequently, this combustion is termed as a "partially sequential auto-ignition" process with the competition determining the local ignition delay between the ϕ -sensitivity effect and the charge cooling effect. In order to realize a sequential auto-ignition process with a further mitigated MPRR, the region 1 in Fig. 8(b) should be avoided by enhancing the mixing after DI, through stronger in-cylinder turbulence, for example

Fig. 8. Local equivalence ratio vs. local temperature for the case of SODI= -52° aTDC at (a) -3° aTDC, (b) 2° aTDC, (c) 4° aTDC.

Fig. 9. Iso-surface of OH mole fraction ($7.8e-7$ in red) and equivalence ratio (left: 0.52 in cyan, 0.43 in blue; right: 0.47 in blue) at 2° aTDC for the case of SODI= -52° aTDC. 1 and 2 stands for the regions 1 and 2 in Fig. 8(b).

Fig. 10. Iso-surface of OH mole fraction ($6.5e-7$ in yellow) and equivalence ratio (left: 0.52 in cyan, 0.43 in blue; right: 0.47 in blue) at 2° aTDC for the case of SODI= -52° aTDC.

In Fig. 11, the local ϕ - T map is plotted with two different crank angles for the case of SODI = -5° aTDC. In Fig. 11(a) at 0° aTDC, only the leanest mixture, mainly from PFI, generates heat release with an HCCI combustion since the richer mixture from DI does not have enough time to ignite at this crank angle. Nevertheless one can see that there is an extensive development of chemical activity in very rich, low temperature regions, following DI. In Fig. 11(b) at 5° aTDC of CA50, the figure is plotted with contours indicating the locations where soot and NO_x formation occur. The zones of soot and NO_x formation are sketched based on the numerical results of n-heptane

by Kitamura et al. [46]. Akihama et al. [47] show that the ϕ - T map has a universal application without fuel-type influence. Although an early phase of CA50 is plotted in Fig. 11(b) when the emission formation and destruction are progressing, the ϕ - T parameter space can be a useful tool for visualizing how the combustion and emissions transiently occur from an overall perspective. First the DI of fuel into the combustion chamber initializes a mixing process, followed by rapid heat release of rich mixture to the flame temperature with little additional mixing. Subsequently, the additional mixing with oxidant or the products of more complete combustion causes the path to follow the mixing-controlled burning. Beyond $\phi = 1$, post combustion mixing serves to lower the temperature. These paths with green arrows in the figure comprise a conventional diesel engine combustion process [48], which means the weak MPRR in this case is relaxed by the slow combustion resulting from the mixing-limited combustion. In the lean side, the black arrows indicate a partially sequential auto-ignition. In this plot, the overlapped region of high NO shows the agreement between the reference data and the simulated results. Though there is no soot model added in the computational work, according to the predictions by Kitamura et al. [46], soot should be at a low level concentration (Fig. 11(b)).

Fig. 11. Local equivalence ratio vs. local temperature for the case of SODI=-5° aTDC at (a) 0° aTDC and (b) 5° aTDC. The scatter contour in (b) is the mole fraction of NO.

7. Conclusions

This paper examines previous experimental observations of Gasoline Compression Ignition (GCI) engine heat release behavior using 3D-CFD and a newly-developed reduced chemical mechanism and gasoline surrogate. A different explanation for the heat release behavior than previously reported is suggested by the CFD results. The major results and findings of the study are:

- A novel 5-component surrogate for a Haltermann 437 certification gasoline (AKI=93) was developed based on the physical and chemical properties of the fuel.
- A 107-species reduced mechanism and a 207-species skeletal mechanism targeted for the 5-component gasoline surrogate was developed from an updated version of the 1389-species LLNL detailed gasoline

surrogate mechanism under GCI engine target conditions. Validation against RCM experimental data and the detailed mechanism shows that the two small mechanisms can predict ignition delay time accurately for the Haltermann 437 certification gasoline under a wide range of engine conditions.

- Using the 5-component certification gasoline surrogate and the 107-species reduced mechanism, two experimental boosted GCI combustion cases with similar MPRR and heat release parameters but very different DI timings are validated and analyzed through 3D RANS simulations. AMR level of 2 (0.5 mm) is determined for the two-case computation by a grid convergence study.
- For the case with DI at -52° aTDC, the GCI combustion can be interpreted as a partially sequential auto-ignition by the competition between the charge cooling effect and the ϕ -sensitive effect for the stratified mixture, which is responsible for the mitigation of the MPRR.
- For the case with later DI at -5° aTDC, the combustion duration is prolonged by the mixing process between the late injected fuel and the well-mixed mixture. The GCI combustion can be decoupled into a partially sequential auto-ignition and a subsequent non-premixed combustion by the late DI near TDC. The weak MPRR is relaxed by the slow combustion resulting from the mixing-limited combustion.

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Table 1

Surrogate formulation

	Volume %	Mole %
$C_6H_5CH_3$	30.9	37
iC_5H_{12}	35.1	27
iC_8H_{18}	24.8	27
nC_5H_{12}	4.6	5
nC_7H_{16}	4.6	4

Table 2

Typical properties of Haltermann 437 gasoline and its surrogate

	HF437	Surrogate
AKI	92.7	91.6
RON	96.6	95.4
MON	88.7	87.8
Sensitivity	7.9	7.6
H/C ratio (mole/mole)	1.81	1.86
Aromatics (vol %)	30.7	30.9
Olefins (vol %)	0.5	0
Saturates (vol %)	68.8	69.1

Table 3

Target conditions in mechanism reduction for GCI engine simulation.

	φ	T [K]	P [atm]
$t_{ign}-1$	0.2	750	10
$t_{ign}-2$	0.2	750	80
$t_{ign}-3$	0.3	800	40
$t_{ign}-4$	0.6	800	10
$t_{ign}-5$	0.6	1100	10
$t_{ign}-6$	0.6	750	60
$t_{ign}-7$	0.6	1000	60
$t_{ign}-8$	1.0	800	10
$t_{ign}-9$	1.0	875	60
$t_{ign}-10$	1.0	750	60
$t_{ign}-11$	2.0	1100	10
$t_{ign}-12$	2.0	700	20
$t_{ign}-13$	2.0	800	40

Table 4

Engine specifications in the experiment.

Displacement	467.5 cc
Compression ratio	15:1
Bore diameter	80 mm
Stroke	93 mm
Connecting rod length	139 mm
Intake valve opening	-363° aTDC
Intake valve closing	-159° aTDC
Exhaust valve opening	134° aTDC
Exhaust valve closing	354° aTDC
Engine speed	1200 rpm
Intake pressure	1.8 bar
Intake temperature	353 K
Coolant temperature	353 K
DI ratio	40%

Table 5Heat release parameters, MPRR, and NO_x emission data validation

	-52° aTDC		-5° aTDC	
	Exp.	Sim.	Exp.	Sim.
CA10 [° aTDC]	3	4.0	2	2.8
CA50 [° aTDC]	5	6.4	4	4.9
CA90 [° aTDC]	7	7.4	10	10.5
MPRR [MPa/ms]	12.5	20.8	15.2	18.6
NO _x [ppm]	<5	44	930	532

Figure1a

Figure1b

Figure1c

Figure2

Figure3

Figure4

Figure5

Figure6

Figure7

Figure8a

Figure8b

Figure8c

Figure9left

Figure9right

Figure10left

Figure10right

Figure11a